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To the problem of the reaction mechanism of 2-methoxybenzo[d]-1,3,2- dioxaphosphorin-4-one with chloral on the basis of quantum-chemical calculations: II. The perkov reaction

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Abstract

The Perkov reaction mechanism on an example of 2-methoxybenzo[d]-1,3,2- dioxaphosphorin---one reaction with chloral was investigated by means of quantumchemical calculations [PM3, DFT (PBE functional, "Triple z" basis, "Priroda" program)]. The primary reaction step is shown to include [1+2]-cycloaddition to form an intermediate with pentacoordinated phosphorus atom (oxaphosphirane-containing spirophosphorane) which transforms further to vinyl phosphate. Structure of the transition state on the pathway to vinyl phosphate is close to dichlorovinyloxyquasiphosphonium cation with the chloride counterion. Thermodynamic parameters of the starting compounds and reaction products as well as activation energies of the processes are evaluated. © Pleiades Publishing, Inc., 2006.

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